

Anisole
100-66-3 | DTXSID4041608

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.61 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.26e-01

Confidence level: 6.88e-01

Nearest Neighbors from the Training Set

Image not found

Styrene

Measured: 3.54

Predicted: 4.53

Image not found

trans-Stilbene

Measured: 1.53

Predicted: 4.45e-03

Image not found

cis-Stilbene

Measured: 1.53

Predicted: 4.45e-03

Image not found

Nitrogen mustard (HN-1)

Measured: 1.66

Predicted: 3.16e-01

Image not found

Tridecane,1-bromo-

Measured: 2.38e-01

Predicted: 1.56e-03

Image not found

1,1-Dimethoxyethane

Measured: 9.25e-01

Predicted: 115